

Theory and Data Analysis for the High Momentum End of ^4He spectrum

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The hybridization of the single-excitation branch with the two-excitation continuum is reconsidered from the theoretical point of view by including the effect of the interference term between one and two excitations. The phenomenological theory presented is used to reproduce the experimental data over a wide region of momentum ($2.3\text{-}3.6 \text{ \AA}^{-1}$) and energy ($0\text{-}12 \text{ meV}$). It is thus possible to extract the final part of ^4He spectrum with higher accuracy. It is found that data agree with a dispersion relation always below twice the roton energy. This is consistent with the negative value of the roton-roton interaction found.

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INTRODUCTION

Excitations in superfluid ^4He have been widely studied in the last decades.¹ However, the nature of the single particle spectrum termination is still unclear. Pitaevskii a long time ago² predicted a termination of the spectrum due to a decay into pairs of rotons. Qualitatively the theory predicts that the low energy pole is repelled by the continuum, so that the spectrum flattens out for large Q towards 2Δ losing spectral weight (Δ is the roton energy). At the same time, a damped excitation for $\omega > 2\Delta$ appears and shifts to higher energies. More precisely, the end of the spectrum is determined by the sign of the roton-roton (V_4) interaction. If this is positive, the spectrum terminates non analytically at 2Δ and at a definite momentum Q_c . On the contrary, if $V_4 < 0$ the spectrum should go smoothly to the two-roton bound state energy slightly below 2Δ . In this second case a sharp peak should survive up to large values of momentum, even if its spectral weight should decrease very rapidly. (This second scenario was proposed by Zawadowski-Ruvalds-Solana³ and Pitaevskii.⁴) In both cases no damping of

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the excitations is possible below 2Δ , nor the *sharp excitation* can exceed 2Δ .

Neutron scattering experiments suggest that the decay of excitations into *pairs of rotons* does actually take place for momentum $Q > 2.6 \text{ \AA}^{-1}$.⁵ Despite the good *qualitative* agreement between theory and experiment the sign of V_4 is still undetermined and the possibility that the excitation energy exceeds 2Δ seems suggested by the data. Direct fitting of Pitaevskii-ZRS theory to data⁶ indicates that $V_4 > 0$, but experimental finding of a quasiparticle peak above 2Δ is not accounted for by the theory with reasonable values of the parameters. As a matter of fact, the position of the quasiparticle energy was extracted by fitting a Gaussian peak on a background of constant slope.⁶ Furthermore, the experimental finding of a (large) positive V_4 , from the theoretical point of view, is completely inconsistent with the observation of a spectrum that does not disappear at any finite Q . Recent experimental investigations by Fåk and coworkers^{7,8} on the temperature dependence of the dynamical structure factor $S(\mathbf{Q}, \omega)$ shows clearly that there is a strong correlation between the low-energy peak and the high energy continuum as Q increases from 2.3 to 3.6 \AA^{-1} .⁸ Thus supporting the hybridization picture.

In this paper we address these inconsistencies that we believe are mainly due to the difficulty of taking properly into account the contribution of the continuum of excitations starting *at* 2Δ , when, for large Q , it becomes more important than the discrete contribution of the sharp state slightly below 2Δ .

1. PITAEVSKII-ZRS THEORIES AND THEIR EXTENSION

We recall that the validity of Pitaevskii and ZRS theories is restricted to a small region around 2Δ . Indeed Pitaevskii in his original paper² exploited the logarithmic divergence appearing in the two-roton response function $[F_o(\mathbf{Q}, \omega) = i \int \frac{d\omega'}{2\pi} \int \frac{d^3\mathbf{Q}'}{(2\pi)^3} \mathcal{G}(p-p') \mathcal{G}(p')]$, where $\mathcal{G}^{-1}(p) = \omega + i0^+ - \omega(\mathbf{Q})$, $\omega(\mathbf{Q})$ is the measured spectrum and $p = (\mathbf{Q}, \omega)$] to solve *exactly* the many-body equations. This elegant theory provides an explicit expression for the Green function valid *only* in the small energy range where the singularity dominates. This fact leads to problems in data analysis when the bare excitation energy $\omega_o(\mathbf{Q})$ reaches values well above 2Δ , since the signal around 2Δ strongly decreases. To understand the correlation between the high energy part of the spectrum and the one-excitation contribution, it is thus necessary to extend the validity of the theory to a wider range of energies in order to describe properly the continuum contribution to $S(\mathbf{Q}, \omega)$. It then becomes crucial to consider the two main channels that contribute to the continuum: The excitation of a quasiparticle that then decays into a pair

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of quasiparticles and the direct excitation of two quasiparticles. It is possible to construct a phenomenological theory that takes into account this two channels. Details are given elsewhere,⁹ here we only report the following simple expression for the density-density response function χ :

$$\chi(p) = \frac{\alpha^2 + 2\alpha\beta V_3 F(p) + \beta^2 F(p) \mathcal{G}_o^{-1}(p)}{\mathcal{G}_o^{-1}(p) - V_3^2 F(p)}. \quad (1)$$

In this expression (valid at zero temperature) α and β are the matrix element for the excitation of one and two quasiparticles, respectively. The coupling V_3 parametrizes the decay amplitude and $F(p)$ is given by the sum of all the diagrams with two lines joined at the two external legs linked at least by two lines.⁹ The effect of a V_4 interaction is completely hidden in $F(p)$, and if we consider only energies near the threshold, Pitaevskii-ZRS theory can be used to obtain an explicit expression for $F(p)$. The dynamical structure factor is simply related to χ by $S(\mathbf{Q}, \omega) = -\text{Im}\chi(\mathbf{Q}, \omega)$ and Eq. (1) constitutes the starting point to analyze data. We also note that Eq. (1) for $\beta = 0$ gives the Green function of one quasiparticle. The above expression thus defines a \mathcal{G} and a χ that share the same poles as expected in a Bose condensed system.¹

2. DATA ANALYSIS AND RESULTS

Since the explicit calculation of F is a difficult task and in general depends strongly on the detailed structure of the vertex functions, we do not try to calculate it microscopically, but we extract it directly from data by exploiting the large (energy and momentum) region of validity of Eq. (1). The main idea is to extract a one-dimensional function $[F(\omega)]$ from a two-dimensional experimental function $[S(\mathbf{Q}, \omega)]$. As a matter of fact the main Q -dependence of Eq. (1) is through $\omega_o(\mathbf{Q})$, since $F(\mathbf{Q}, \omega)$ is expected to depend weakly on \mathbf{Q} (as is the case for $F_o(\mathbf{Q}, \omega)$ in this momentum region). It is thus possible to extract $F(\omega)$ and $\omega_o(\mathbf{Q})$ by fitting Eq. (1) to the different sets of data with different momentum *at the same time*. This procedure exploits fully the information contained in the data because it is sensitive to the correlation among sets with different Q .

To extract the complex function $F(\omega)$ from data we parametrize its imaginary part with N real numbers (15 in the fit presented) in the following way. We choose a set of values of ω , say $\{\omega_1, \omega_2, \dots, \omega_N\}$ with $2\Delta = \omega_1 < \omega_2 < \dots < \omega_N$ reasonably spaced and we assign a *free* parameter, a_i , to each of them. $\text{Im}F(\omega)$ can then be defined as a cubic spline interpolation on such a set. The real part can then be easily obtained by the relation $\text{Re}F(\omega) = -1/\pi\mathcal{P} \int d\omega' \text{Im}F(\omega')/(\omega - \omega')$. It is also important to reduce

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the parameters to the minimum number of independent ones, so we define a dimensionless function $f(\omega) = \lambda F(\omega)$, constrained by the normalization condition $\int_{2\Delta}^{\omega_N} d\omega \text{Im} f(\omega) = \omega_N - 2\Delta$, and $g_3 = V_3/\lambda^{1/2}$, $\tilde{\beta} = \beta/(\lambda^{1/2}\alpha)$. In this way α , β , g_3 , and the $N - 1$ parameters that define f are independent and can be fitted to the data.

We thus fitted Eq. (1) (convolved with the known instrumental resolution) to experimental data of Ref. 8 at 1.3 K. The resulting fit is shown in Fig. 1. The good agreement between theory and experiment is obtained with a reduced χ^2 of nearly 4, thus indicating that even if we are leaving a large freedom in f the agreement is significant.

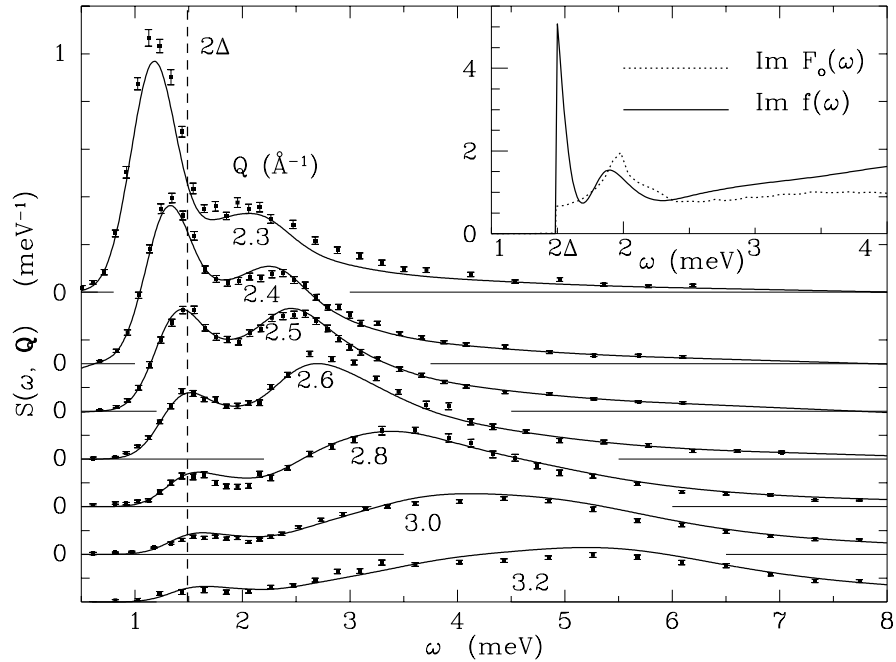


Fig. 1. Fit to the data from Ref. 8 with a parametrized $\text{Im}f$. In the inset the resulting $\text{Im}f$ is shown compared with $\text{Im}F_o$ averaged over $2.3 < Q < 3.2 \text{ \AA}^{-1}$ and properly scaled.

The new dispersion relation for the undamped excitation is reported in Table 1. Note that the value of 2Δ is 1.484 meV .¹⁰ The fitted values of the normalized a_i is also reported in Table 1.

We find that the model can *quantitatively* explain that the peak position of $S(Q, \omega)$ is slightly larger than 2Δ for $Q > 2.6 \text{ \AA}^{-1}$. This originates from

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Q \AA^{-1}	$\omega(Q)$ meV	$Z(Q)$	$\omega_o(Q)$ meV	ω_i (meV)	
				ω_i (meV)	a_i
2.3	1.174 ± 0.005	0.372 ± 0.019	1.42	1.484	2.7
2.4	1.303 ± 0.003	0.234 ± 0.025	1.88	1.56	1.10
2.5	1.381 ± 0.002	0.133 ± 0.019	2.4	1.68	0.33
2.6	1.420 ± 0.005	0.075 ± 0.008	2.8	1.75	0.45
2.8	1.455 ± 0.010	0.031 ± 0.005	3.7	1.85	0.71
3.0	1.467 ± 0.008	0.017 ± 0.002	4.6	2.00	0.63
3.2	1.473 ± 0.010	0.011 ± 0.001	5.3	2.15	0.44
3.6*	1.480 ± 0.010	0.003 ± 0.001	6.8	2.50	0.44
				3.0	0.57
				3.5	0.67
				4	0.78
				5	0.88
				6	0.97
				9	1.35
				12	1.09

Table 1. Dispersion relation for the quasiparticle spectrum, weight ($Z(Q)$) of the pole, and energy of the bare pole ω_o (left Table). Fitted values for a_i at each ω_i (right Table). The values for $Q = 3.6 \text{ \AA}^{-1}$ are obtained from a fit not shown.

a mixing within the instrumental resolution of the contribution of the sharp peak at energy ω_Q slightly smaller than 2Δ with that of the continuum of two rotons excitations starting at 2Δ . On general grounds the continuum should depend strongly on ω near 2Δ , as for $\omega > 2\Delta$ there are much more states available to decay into. Our procedure exploits the theoretical model for $\chi(p)$ to extract both the value of ω_Q and the continuum contribution. In this way we can find the final part of the dispersion relation with improved accuracy. It turns out that data agree with a dispersion relation for the excitations always below 2Δ .

Concerning the other parameters of the fit we find $\alpha^2 = 1.4$, $\tilde{\beta} = -0.06 \text{ meV}^{-1/2}$ and $g_3 = 0.8 \text{ meV}^{1/2}$. This implies that the direct excitations of two quasiparticles by the neutron gives a small but *appreciable* contribution to $S(\mathbf{Q}, \omega)$, particularly at high energy.

The shape of $\text{Im}f$ found with the fit (see Fig. 1) has two main features: A clear peak at $\omega \approx 2 \text{ meV}$ and a “quasi-divergent” behavior at the threshold. The peak is due to the maxon-roton van Hove singularity as is clear by comparison with F_o . It is remarkable that although no trace of the peak is apparent in any of the experimental plots the procedure succeeded in finding correctly this information.

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The quasi-singularity at threshold can be understood as an interaction effect, namely a signature of the roton-roton attractive interaction. As a matter of fact, in the *small region* of energy near the threshold we can apply Pitaevski-ZRS theory to evaluate $F(\omega)$. We verified quantitatively this fact by repeating the fit using Pitaevskii-ZRS theory to parametrize $f(\omega)$ and setting a cutoff in energy at $2\Delta+0.2$ meV. The resulting reduced χ^2 for the fit gives evidence that the theory works *quantitatively* in this small region. We obtained in this way for the interaction parameter $V_4 \approx -4.7$ meV \AA^3 with a tiny bound-state energy of $1.3 \mu\text{eV}$. Note that without the cutoff this theory is not able to fit data satisfactorily.

In conclusion, we presented a theory for $S(\mathbf{Q}, \omega)$ that takes into account both one- and two-quasiparticle excitations by the neutron. The theory reproduces the experimental results over a large range of energy and momentum. We have thus been able to extract the final part of the spectrum dispersion relation in ^4He and to determine its end as an hybridization with the bound state of two rotons.

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REFERENCES

1. See for instance: A. Griffin, *Excitations in a Bose-Condensed Liquid* (Cambridge University Press, Cambridge, UK, 1993). H. R. Glyde, *Excitations in Liquid and Solid Helium* (Oxford University Press, Oxford, UK, 1994).
2. L. P. Pitaevskii, Sov. Phys.-JETP **36**, 830 (1959).
3. J. Ruvalds and A. Zawadowski, Phys. Rev. Lett. **25**, 333 (1970). A. Zawadowski, J. Ruvalds, and J. Solana, Phys. Rev. B **5**, 399 (1972). K. Bedell, D. Pines, and A. Zawadowski, Phys. Rev. B **29**, 102 (1984).
4. L. P. Pitaevskii, JETP Lett. **12**, 82 (1970).
5. R. A. Cowley and A. D. B. Woods, Can. J. Phys. **49**, 177 (1971).
6. A. J. Smith *et al.*, J. Phys. C **10**, 543 (1977).
7. B. Fåk and K. H. Andersen, Phys. Lett. A **160**, 469 (1991). B. Fåk, L. P. Regnault, and J. Bossy, J. Low Temp. Phys. **89**, 345 (1992).
8. B. Fåk and J. Bossy, J. Low Temp. Phys. in press (1998).
9. F. Pistolesi, submitted to Phys. Rev. Lett.
10. R. J. Donnelly, J. A. Donnelly, and R. N. Hills, J. Low Temp. Phys. **44**, 471 (1981).